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Has the Time Come for Preprints in Chemistry?

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ABSTRACT: Chemistry is among the last of the core natural sciences to embrace preprints, namely, the publication of non peer-reviewed scientific articles on the Internet. After a brief insight into the origins and the purpose of preprints in science, we conducted a concrete analysis of the concrete situation, aiming at providing an answer to several questions. Why has the chemistry community been late in embracing preprints? Is this in relation with the slow acceptance of open-access publishing by the same community? Will preprints become a common habit also for chemistry scholars?

1. INTRODUCTION

Communities of computer scientists started to share documents via computer networks in the 1970s.[1] Yet, prepublication of scientific research as we know it today, namely, the act to share online a scientific article (a preprint) before the peer-review process, debuted in the physics community in 1991 when Ginsparg, a physicist at Los Alamos National Laboratory in the United States, released software to share drafts of articles via e-mail transactions referring to a central repository online.[2] Calling them "preprints", as noted by Bourne and colleagues recently,[3] is an anomaly of language as most of these documents will never have a print version but only a digital one and most often a digital object identifier (DOI) alphanumeric string.

With preprints, scholars retain the author rights prior to publication and can subsequently publish their work in any journal accepting preprint manuscripts. Preprints, in general, are stably archived, dated, and citable, thereby providing evidence for research activity.[4]

With the advent of World Wide Web, the repository for physics articles was first migrated to http://xxx.lanl.gov and then to http://arXiv.org, a website managed by the Library of Cornell University. As of June 2017, arXiv hosted more than 1.27 million articles in the fields of physics, mathematics, computer science, quantitative biology, quantitative finance, and statistics, with over 120 000 new submissions expected in 2017.[1]

In late 2013, it was biologists' turn, with the launch of http://bioRxiv.org, a repository for the life sciences research community hosted, again in the US, by Cold Springer Harbor Laboratory. From publishing 824 preprints in the first year,[5] the website has grown to current 1000 monthly submissions,[6] with over 12 000 preprints already archived. In 2016, the engrXiv, SocArxiv, and psyArXiv platform were launched to serve, respectively, the engineering, social sciences, and psychology communities. So significant has become the impact of preprints that in 2016 two preprints (the 21st and 28th entries, respectively, from bioRxiv and PeerJ Preprints) were in the top 100 list of the most-discussed journal content of the year as reported by Altmetric.[7] More importantly, as emphasized by the founder of arXiv,[2] Perelman's proof of the Poincaré conjecture in three dimensions, for which the Russian mathematician was awarded the Fields Medal in 2006, appeared only in three remarkable preprints published in arXiv in 2003. Similarly, Greider regularly publishes her findings in bioRxiv along with other Nobel Prize laureates.

As of July 2017, the Open Science Framework free service had indexed more than 2 million preprints from several disciplines, in fields ranging from architecture to law to education, from preprint repositories (within brackets the number of preprints) such as AgriXiv (12), arXiv (1 209 405), bioRxiv (12 455), BITSS (9), Cogprints (263), engrXiv (115), LawArXiv (194), LIS Scholarship Archive (5), MindRxiv (1), PeerJ (2235), http://Preprints.org (1765), PsyArXiv (649), RePEc (804 006), and SocArXiv (1259). Similarly, the Brazilian online publishing platform SciELO announced in early 2017 a forthcoming preprint service.[8]

In chemistry, the preprint server *Nature Precedings* launched in 2007 was closed in 2012 as the website had become "unsustainable as it was originally conceived".[9] A similar fate was shared by the chemistry preprint server launched by Elsevier in 2000 (along with those in mathematics and computer science) and closed in early 2004 as "the Chemistry, Maths, and Computer Science research communities did not contribute articles or online comments to the Preprint service in sufficient numbers to justify further development".[10] Thirteen years later, in 2017, Elsevier launched ChemRN,[11] a chemistry preprint server managed through a leading social

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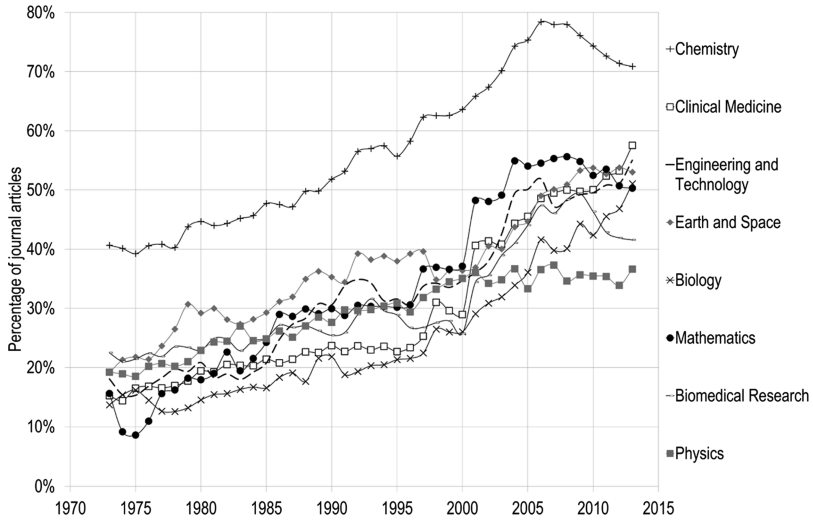

Figure 1. Percentage of papers published by the five major publishers by discipline in the natural and medical sciences, 1973−2013. [Reproduced from ref 15, with kind permission].

science and humanities online repository acquired the year before. A few days later, ChemRxiv, the preprint server announced in 2016 by the American Chemical Society (ACS),[12] was released in a fully functioning "beta" release, a remarkable change compared to 2000 when, with the launch of Elsevier's chemistry preprint server, "nearly all ACS journal editors lined up against it".[13]

Hosted by the ACS and coordinated with inputs from the ACS, the Royal Society of Chemistry (RSC), the German Chemical Society (GDCh), the broad chemistry community, and other not-for-profit groups and scientific publishers, ChemRxiv made its debut in August 2017 publishing a theoretical work on "excitonics", namely, binary gates for molecular exciton processing and signaling.[14]

Why has the chemistry community been late in embracing preprints? Is this related to the slow acceptance of open-access (OA) publishing by the same community? Can we expect widespread acceptance of preprints also from chemistry scholars? This study aims to give an answer to these and related questions. After a brief insight into the origins and the purpose of preprints in science, we conducted an analysis of the situation, offering an insight into a topic of direct relevance to today's and tomorrow's practitioners of chemical research.

2. ANALYSIS

An analysis of preprints in chemistry should start with a consideration of the economic relevance of the global scientific publishing industry.[15] This had global revenues in 2016 exceeding $24.6 billion, with some company's profits potentially exceeding a 35% margin.[16]

From the publishing viewpoint, chemistry is unique among natural sciences because 80% of chemistry papers published in 2006 were published by the five major natural and medical science publishers (ACS, Reed-Elsevier, Wiley-Blackwell, Springer, and Taylor & Francis). The fraction was still above 70% in 2013, whereas it was 40% in 1973 (Figure 1). In the physics community, for comparison, the proportion of papers published in 2013 by the top five publishers was about 35%.[13]

So far, attempts by public funding agencies to encourage researchers receiving public money to publish their research findings as OA articles mostly have not been met with universal success. Notably in 2017, the Gates foundation began to require all funded researchers to publish papers uniquely in OA format,[17] thereby excluding journals such as *Nature*, *The New England Journal of Medicine*, *Science*, and the *Proceedings of the National Academy of Sciences*. Many other funders have other OA requirements.

In the early 1990s, the advent of the Internet first, and of the World Wide Web later, offered an unprecedented opportunity to scholarly communities, such as immediate posting of their findings prior to peer review, thus bypassing the time to reveal new findings through peer review, where a manuscript may be delayed by successive rejections and resubmissions.[18] Preprints have the intrinsic ability to solve the main problem of the peer-review process, such as a delay in publication. Such delays can be a significant challenge. Some authors are concerned about a refereeing bias, against authors from emerging bylines, or when authors propose ideas different from the mainstream.[19] It is perhaps not surprising that the need for a national preprint repository was first identified for a huge and rapidly developing country such as India, urging young minds to preprint their work on the new national online archive to ensure priority.[20]

By reducing time for publication, preprints enable researchers to establish priority and, at the same time, share results and data with their colleagues. In similar cases, such as Preprints, ChemRxiv, and bioRxiv, the preprint is immediately assigned a DOI which allows citation and citation tracking. Reducing the time for publication can be of vital importance in case of health emergencies, for instance, when research on the Zika virus was publicly made available in real time on the Zika Open-Research Portal (https://zika.labkey.com) to help facilitate collaborative research and move science ahead rapidly toward cures and prevention.[10]

Scholars who post preprints position their research so that colleagues and other scientists around the world can immediately give feedback, helping to progress the work faster. The comments received by other scholars can be used to revise and improve the quality of the work, which often then ends up published in conventional scientific journals, as it happens to a significant fraction of manuscripts posted on arXiv, bioRxiv, and the other repositories mentioned above. Hence, in principle, the fundamental advantage of preprints is the acceleration of scientific and technical progress.

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Another key advantage for authors is that they are able to claim priority on new ideas in preprints. Such postings should help authors avoid having unethical referees take ideas and claim them for their own, an issue lamented by several authors and a known misconduct for which the Committee on Publication Ethics (a body established in 1997 by a group of journal editors now having over 10 000 members worldwide from all academic fields) has published guidelines already in 2010.[21] However intolerable, this practice continues to occur even when submitting to high-impact-factor journals in all sort of disciplines including medicine,[22] and not only to scientists in their early career, as Noble Prize Lipscomb remarked several years ago:

"I no longer put my most original ideas in my research proposals, which are read by many referees and officials. I hold back anything that another investigator might hop on and carry out. When I was starting out, people respected each other's research more than they do today, and there was less stealing of ideas."[23]

Wiersma, a professor of forest resources in the US and the editor of *Environmental Monitoring & Assessment*, argues that the problem with peer review is that it is an "honor system" in which "if people want to break the honor system, there is nothing you can do".[24]

Today, the problem of stealing ideas by unethical referees can be entirely circumvented by the adoption of preprints. Further, key funding agencies supporting research in life sciences, chemistry, and medicine including the National Institutes of Health (NIH) in the US,[25] the UK Medical Research Council,[26] and the Wellcome Trust[27] almost concomitantly announced in early 2017 new policies for which the citation of preprints in grant applications is accepted and, in some cases, encouraged.

Research chemists have been notoriously reluctant to accept OA, and the number of OA publications in chemistry is still significantly lower than those in many other disciplines.[28] Puzzled by such low response of the chemistry community, scientific information scholars have advanced all sort of tentative explanations: from chemistry being a "long tail" science in which small research units would adopt a predominantly noncollaborative mode of research,[29] through the influence of the chemical industry and proprietary information.

In a presentation given at the 2011 Spring Meeting of the ACS, the editors of the first scientific OA publisher in chemistry (Chemistry Central, founded in 2006, whose parent company BioMed Central was acquired two years later by Springer), noting that the acceptance of OA in chemistry was 5 years behind life sciences, suggested one of the main reasons:[30] the influence of chemical societies, three of which (ACS, RSC, and GDCh) are among the leading publishers in chemistry today publishing several OA journals.[31]

In detail, the team showed the outcomes of the European Union-funded Study of Open Access Publishing involving 42 000 respondents and 2300 chemists across the world in which the lowest percentage of researchers who said that OA journals would be beneficial were chemists.[32] In the ranking by country, research chemists based in the UK (31st out of 33 countries), in the US (24th), and in Germany (19th) were in the lower part of the ranking.

Interested in their career and in securing funds for their research, chemists continue to publish in journals of renowned reputation so as to increase the impact of their research in terms of citations and thus their h-index and other scientometric indicators to which their promotion and tenure track are closely bound,[33] although studies showing that OA articles, for example, in computer science receive significantly more citations than subscription-based articles that appeared in prestigious journals as early as of 2001.[34] Furthermore, academic review committees often use publication count and the "quality" of journals published in to evaluate people much more than citation count. Put bluntly, "a paper in a poorly known journal which is cited 200 times is worth much less than a *Nature* paper which is cited three times".[35] Yet, as the third decade of the 21st-century approaches, the use of preprints might become the norm also in chemistry, as we critically aim to argue in the following.

3. DISCUSSION

In the last two decades, two significant changes have occurred in communicating chemical research. One is the now complete digitalization of the scientific information flow,[36] with several chemistry journals no longer printing journal issues but producing only articles in digital format (normally in both portable document format and hypertext markup language). Another is the now predominant use of the World Wide Web to search for scientific information,[37] especially through free search services such as those offered by Google Scholar. The latter search engine, furthermore, effectively tracks citations of researchers who use it also for locating updated scientometric information of relevance to their own research interests.[38]

From *Chemical Communications* to *Organic Letters*, numerous prestigious journals are available to chemists to quickly publish findings of high relevance, and even in OA format when paying the article publishing charge. The same is true for biology and physics where numerous journals, including new "express", "protocols", and "letters" versions of prestigious titles, offer a fast track to peer-reviewed publication, but this has not slowed down the acceptance of preprints in those communities. In our view, scholars in the chemical sciences will likely soon start to use preprints to claim priority for their findings, sharing, and collecting feedback in matter of days or weeks, rather than in months or years as it used to be with conventional publishing. For those who stick to the old model, the risk is to see colleagues posting preprints of their work in the same subfield of contemporary chemical research to rapidly progress the field while they are still waiting months for the reviewers' reports.

This is also the case of what happened in the biology community, which came to preprints about two decades after physics. An information specialist arguing in early 2016 that they were curious "to see if bioRxiv continues to see its submissions grow",[10] one year later saw the number of preprints in bioRxiv surpassing the 12 000 threshold (from less than 900 in the first year).

This may explain why large publishers have recently started new preprint repository services, such as preprints owned by MDPI, and it may also explain why arXiv[39] and bioRxiv[40] were frequently used also by chemists, often for preprints jointly authored with physicists or life scientists. Gone are the days when chemistry preprint servers were being closed owing to insufficient submissions.

Joining the open science practice, chemists and especially young chemical research practitioners will discover or rediscover that, as stated by Nosek, a social psychologist and open science advocate, "sharing is good", that is, sharing research with peers is good for discovery,[41] thus restoring the original

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meaning of scientific publication vividly illustrated by Evariste Galois, the eminent mathematician creator of the Group theory (later widely used by theoretical chemists), in 1831:

"Je rêve d'un temps où l'égoïsme ne régnera plus dans les sciences, où on s'associera pour étudier, au lieu d'envoyer aux académies des plis cachetés, on s'empressera de publier ses moindres observations pour peu qu'elles soient nouvelles, et on ajoutera: "Je ne sais pas le reste" (I dream of a time when selfishness will no longer reign in the sciences, when people will associate to study, instead of sending sealed folds to the academies, hastening to publish their least observations no matter of carrying just a bit of innovation, adding: "I do not know the rest")".[42]

Whether or not preprints and OA will rid science of egoism, as auspicated by Galois, interest for claiming priority, gaining visibility, and eventually securing research funds perhaps will become more powerful drivers for this movement.

Following the recent decision of the world's largest science funding agency (NIH, funding research with >$26 billion in 2013),[43] we can reasonably anticipate that other scientific funding agencies worldwide will approve citation of preprints in grant applications, including those supporting research in chemistry. Following such acceptance by funders, promotion, search, and tenure committees will do the same, accepting the citation of preprints in the curriculum of applicants. We expect, as with NIH,[44] this will occur, along with adopted clear policies on how preprints should be evaluated and what types of preprint servers should be used. In another recent example of emerging guidelines for preprint servers, the director of the GDCh noted "nonrefereed publications, for example on preprint servers, should be clearly classified as such".[45]

4. CONCLUSIONS

This work aims to answer the question whether the time has come for preprints in chemistry, as compared to the analysis by geneticist Bhalla for biology preprints in early 2016.[46] The study mainly compares the special case of chemistry with biology, as a natural science discipline that has recently embraced preprints.

Although being among the last core natural sciences to embrace preprints, chemistry is poised for success in this evolution. Interested in their career and securing research funds, chemistry researchers cannot ignore preprints any longer. Preprints are accepted and even encouraged by public funding agencies, starting from the world's largest (the NIH), and are soon expected by many others across the world. Many preprints are fully indexed; preprints are widely read (as of mid-September 2017, the first six preprints in BioRxiv had 408 384 downloads, with the sixth alone counting 26 367 downloads),[47] and cited (e.g., preprints in the arXiv condensed matter section were found in 2006 to be cited nearly twice more than nonpreprinted publications),[48] providing researchers with the visibility in the research community while enabling authors to easily access online the article metrics and be contacted by interested collaborators or fellow scientists.[49]

From the fundamental viewpoint of research practice, the benefits of immediate feedback on the preprint from a much wider audience (online preprints can be freely accessed and downloaded) are so significant that scholars competing for priority in discovery and innovation will increasingly post their findings as preprints as a normal part of the research communication process. Preprints, indeed, have the intrinsic ability to add value to the peer-review process.[50]

One might also ask what role will scientific journals play when every paper is posted as a preprint, namely, what value would journals add in such a scenario. Typically, part of the value assigned to journals is their editing and peer-review processes.[51] Both services can now be obtained for prepublication work. For peer review, for example, F1000Research transforms a preprint in a published article after it is openly peer-reviewed and accepted; for editing, authors can hire a scientific editor for a particular article without involving a journal. Therefore, basically, if this scenario will materialize, today's journals will reshape into online publication platforms publishing first the preprint (following a first editorial scrutiny) and then, following renewed peer review, publishing the OA final version of the article linked with the preprint.

Eventually, preprints will help to provide a mechanism to move the field toward a new publishing model where each work stands on its own merits regardless of what journal it is published in. This is what happened in physics arXiv and in biology with bioRxiv, where even the sole prepublication of the proof of the Poincaré conjecture in three dimensions granted Perelman in 2006 the equivalent of Nobel Prize in mathematics. Also in chemistry, journal editors will start browsing preprint servers looking for suitable articles likewise to what the editors of *PLOS Genetics*[52] and *Genome Biology*[53] currently do, soliciting authors to submit their preprints for peer review and, increasingly, for open peer review.

To compete with numerous prestigious journals such as *PLoS One* accepting preprints, chemistry journals which currently do not accept preprints will shortly be pressurized to change their policies toward prepublication, as it already happened at the majority of chemistry journals. ACS journals, for example, have set prior publication policies, including whether to accept or reject preprints. As a sign of the growing acceptance of preprints in the chemistry community, the majority of the latter journals now allow preprints.

At the 2017 Lindau Meeting of Nobel Laureates, Chalfie lately informed the audience that periodically a member of his research group is required to select a preprint on a topic related to his/her research.[54] The study is discussed in a subsequent group meeting, and comments are eventually sent to the corresponding author of the preprint to raise new ideas both in Chalfie's group and in that of the author.

Why should research groups in chemistry not adopt similar practices? Chemists also are clearly interested in adopting a more collaborative mode of research which makes use "of new technologies to facilitate data sharing and research collaboration".[29]

In China, where chemistry in 2014 accounted for 61% of the country's total weighted fractional count,[55] collaborations in the field of chemistry soared to unprecedented levels, with major collaborations in 2015 with groups based in the US, Germany, Japan, Singapore, UK, Australia, Canada, and France.[56]

Preprint servers will of course need to be supported financially; hence, they will be owned or coordinated by nonprofit scientific societies (such as ChemRxiv with ACS, RSC, and GDCh), existing commercial publishers (such as Preprints or ChemRN), public or private universities (such as arXiv which is principally hosted by the Cornell University Library with financial support from many different organizations including the Simons Foundation), private laboratories (such as bioRxiv principally hosted by the Cold Spring Harbor Laboratory, a private, nonprofit institution), or public or private research funders. Preprint servers will continue to thrive and

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improve, becoming of central relevance and providing a new way to communicate innovation in science, including chemistry. The process of innovation in communication is already underway, and this study will hopefully assist research chemists in the transition to open science for the benefit of the main users of chemical innovation: mankind.

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Notes

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